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Ali Ayoubikaskooli

Islamic Azad University of Gachsaran

Abdol Mohammad Ghaedi

Islamic Azad University of Gachsaran

Hamid Reza Shamlouei (✉ shamlouei.ha@lu.ac.ir)

Lorestan University <https://orcid.org/0000-0002-6842-9685>

Yadollah Saghapour

Islamic Azad University of Gachsaran

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Improving the electrical and optical properties of C50 fullerene using the Donor-Acceptor groups

Ali Ayoubikaskooli¹, Abdol Mohammad Ghaedi¹, Hamid Reza Shamlouei^{2*}, Yadollah Saghapour¹

¹Department of Chemistry, Gachsaran Branch, Islamic Azad University, Gachsaran, Iran

²Chemistry Department, Lorestan University, Khorramabad, Iran

* Corresponding Author: Shamlouei.ha@lu.ac.ir

Abstract

In this research, the C_{50} fullerene was employed as the source of the π electrons and the electron donor-acceptor groups were used to enhance its optical properties. Considerable enhancement in its electronic and optical property of as the result of donor and acceptor group presence was observed. For instance, in UV-Visible absorption spectrum, the number of absorption lines significantly increase which may be the relaxation of the electronic transition selection rules. Considerably, the substituted forms of C_{50} , has numbers of absorption bands in near infrared region. The $BH_2-C_{50}-NCH_3Li$ and $NO-C_{50}-NCH_3Li$ molecules have superior improvement in optical properties. Finally, the donor and acceptor groups influence on non-linear optical properties (NLO) of C_{50} were explored and the considerable improvement in NLO properties of C_{50} was observed which the NLO improvements for $BH_2-C_{50}-NCH_3Li$ and $NO-C_{50}-CH_2Li$ cases is higher than others.

Keywords: Photosensitizer, Fullerene, UV-Visible, NLO

1. Introduction

The photosensitizers are known as molecules that may be used to cause photochemical changes in other molecules [1]. Common uses of photosensitizers may be listed as the hydrogen production process [2-3], polymerization by light [4-5], degradation of material by light [6-7], Dye-sensitized solar cells [8-11], triplet excited states creation in organic molecules [12-13], photodynamic therapy [14-15], *etc.* Absorption of ultraviolet or visible light and its transmission to adjacent molecules is an important feature of photosensitizers. They usually have large delocalized π -framework that lowers the energy of absorbed light. Due to their very pricey syntheses, extensive usages of the porphyrin molecules, as the most known types of photosensitizers, were decreased. Clearly discovering new classes of material with desired properties as alternative of porphyrin molecule may be beneficial.

In previously published researches, two [14] annulene and [26] annulene molecules were suggested as photosensitizers and by using the donor and acceptor groups their optical properties were improved [16-17]. Other options with a delocalized π -framework for use as photosensitizers are [5] circulene and [7] circulene molecules, which had been tried to improve their optical properties with electron donor and electron acceptor groups [18-19].

The fullerenes molecules or C_{60} , which the first member of the fullerene, was first discovered in 1985 [20], can be consider as the good resources of de-localized π -electrons. The C_{60} molecule is a spherical cage containing 12 pentagons and 20 hexagons. The special properties of the C_{60} molecules have attracted scientists to other types of fullerenes [21]. Generally, other types of fullerenes contain twelve pentagons and different numbers of hexagons. They commonly are highly sensitive to light which variations in the wavelength of light influence the electrical property of these materials. Therefore, it is hoped that these materials will

be used, especially in future of photonic applications [22-24]. In present work the C₅₀ fullerene was selected and was used as a source of π -electrons. Improving the electrical and optical of it by the donor and acceptor groups was studied.

2. Computational detail

All structures of considered molecules were optimized using B3LYP methods exchange and correlation functional with 6-311 g(d) basis set. All calculation employed using Gaussian09 package [23]. The electronic density of state for all optimized structures was done using GaussSum03 [24]. Gap energy (E_g) was calculated based on DOS results:

$$E_g = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (1)$$

where E_{HOMO} is the energy of highest occupied molecular orbital (HOMO) and E_{LUMO} is the energy of lowest unoccupied molecular orbital (LUMO). Electronic absorption spectra of all structures were calculated using two TDB3LYP methods exchange and correlation functional with 6-311 g(d) basis set. For study the effect of donor and acceptor groups, different groups was chosen and the fullerene C₄₀ molecule was sandwiched between them. For electron donor substitutions, the -CH₂Li, -NCH₃Li, -NHLi and -CN, -NO, -BH₂ for electron acceptor, groups was used. The energy of a system in the weak and homogeneous electric field can be defined as [25-26]:

$$E = E^0 - \mu_{\alpha} F_{\alpha} - 1/2 \alpha_{\alpha\beta} F_{\alpha} F_{\beta} - 1/6 \beta_{\alpha\beta\gamma} F_{\alpha} F_{\beta} F_{\gamma} - \dots \quad (2)$$

where E^0 is the total molecular energy without the electric field and F_{α} is the electric field component along α direction. In addition, the μ_{α} , $\alpha_{\alpha\beta}$, and $\beta_{\alpha\beta\gamma}$ denote dipole, polarizability, and hyperpolarizability, respectively. The polarizability (α) and first hyperpolarizability (β^0) are expressed as:

$$\alpha = 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (3)$$

$$\beta^o = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2} \quad (4)$$

In which

$$\beta_i = 3/5(\beta_{iii} + \beta_{ijj} + \beta_{ikk}) \quad i, j, k = x, y, z \quad (5)$$

where β^o is the first hyperpolarizability, which is a third rank tensor and known as a nonlinear optical response (NLO) coefficient. The values of polarizability (α) and first hyperpolarizability (β_o), which are representative of linear and nonlinear optical properties of nanotubes, were calculated using a 6-311G (d,p) basis set and CAM-B3LYP method.

3. Result and discussion

3.1 Structural optimization

The structures of C50 fullerene and sandwiched forms of it between the BH2 and NO groups and NHLi, CH2Li and NCH3Li groups as electron donor and acceptors respectively were calculated at B3LYP/6-311G(d,p) computational level. Their optimized structures are illustrated in Fig 1.

C_{50}

$BH_2-C_{50}-CH_2Li$

$BH_2-C_{50}-NHLi$

$BH_2-C_{50}-NCH_3-Li$

$NO-C_{50}-CH_2Li$

$NO-C_{50}-NHLi$

NO-C₅₀-NCH₃Li

Fig 1. Optimized structures of C₅₀ fullerene and sandwiched forms of it between the electron donor and acceptors groups

After calculation the optimized structures of the considered molecules, the first IR frequencies were calculated which first three frequencies of them were reported in Table 1.

Table 1: calculated first three frequencies for C₅₀ fullerene in pristine form and sandwiched form

FORMULA		First three frequencies		
BH ₂ -C ₅₀ -CH ₂ Li	40.75	94.64	104.28	
BH ₂ -C ₄₀ -NCH ₃ Li	74.67	91.80	109.07	
BH ₂ -C ₄₀ -NHLi	75.65	94.02	106.35	
NO-C ₄₀ -CH ₂ Li	28.00	40.02	79.26	
NO-C ₄₀ -NCH ₃ Li	32.46	74.71	92.45	
NO-C ₄₀ -NHLi	30.93	67.75	88.40	

As the result of Table 1, no imaginary frequency was observed in calculated IR spectrum and therefore the existence of transition state was rejected. This is one of the important evidence of molecular stability.

3.2. Electronic Properties

The density of states (DOS) spectrum of pristine form of C_{50} and sandwiched form of it between the donor and acceptor groups were calculated and presented in Fig 2.

C_{50}

$BH_2-C_{50}-CH_2Li$

$BH_2-C_{50}-NCH_3Li$

$BH_2-C_{50}-NHLi$

NO-C₅₀-CH₂Li

NO-C₅₀-NCH₃Li

BH₂-C₅₀-NHLi

Fig. 2 . Calculated DOS spectrum of C₅₀ fullerene and substituted forms of it

In the DOS spectrum, the higher the intensity in each energy shows the higher the density of the electron states. In forbidden region, which located between the HOMO and LUMO has no electronic state. Using the DOS spectra, the energies of HOMO and LUMO were calculated. In

Table 2, the results of ϵ_{HOMO} , ϵ_{LUMO} and E_g for fullerene in pristine form and sandwiched form were reported.

Table2: the results of ϵ_{HOMO} , ϵ_{LUMO} and E_g for fullerene in pristine form and sandwiched form

FORMULA	ϵ_{HOMO}	ϵ_{LUMO}	E_g (eV)
C_{50}	-5.87	-4.56	1.31
$\text{BH}_2\text{-C}_{50}\text{-CH}_2\text{Li}$	-5.39	-3.90	1.49
$\text{BH}_2\text{-C}_{50}\text{-NCH}_3\text{Li}$	-5.09	-3.76	1.33
$\text{BH}_2\text{-C}_{50}\text{-NHLi}$	-5.27	-3.73	1.54
$\text{NO-C}_{50}\text{-CH}_2\text{Li}$	-5.50	-4.04	1.46
$\text{NO-C}_{50}\text{-NCH}_3\text{Li}$	-5.22	-3.92	1.30
$\text{NO-C}_{50}\text{-NHLi}$	-5.37	-3.88	1.49

As illustrated in Table 2, it was shown that the fullerene sandwiched between the donor and acceptor groups increase the energies of both HOMO and LUMO orbitals however, increment in the LUMO orbital is higher than the HOMO orbital. Therefore, in most of the cases the values of E_g increase. Just in $\text{NO-C}_{50}\text{-NCH}_3\text{Li}$ reduction of E_g was observed. The highest value of E_g was obtained for $\text{BH}_2\text{-C}_{50}\text{-NHLi}$. In Fig 3, the E_{HOMO} , E_{LUMO} and E_g was plotted for all mentioned molecules.

Fig. 3: the plot of E_{HOMO} , E_{LUMO} and E_g for all mentioned molecules.

In Fig 3 also variation of E_{HOMO} , E_{LUMO} and E_g for all considered clusters is depicted. As shown donor and acceptor groups presence drastically increase the HOMO energy of the C_{50} . However the value of the E_g in all cases (except $\text{NO-C}_{50}\text{-CH}_2\text{Li}$) increased. The E_g increasing may be the result of the push pull effects of the donor and acceptor groups.

3.3. Optical Properties

To understand the effect of these electron donor and electron acceptor groups on optical properties of C_{50} fullerene, the TDDFT calculation was used to obtain the UV-Visible absorption spectra of all structures. In Fig 4, the UV-Visible absorption spectra of pristine C_{50} fullerene and sandwiched form of it were reported.

C50

BH2-C50-CH2Li

BH2-C50-NCH3Li

BH2-C50-NHLi

NO-C50-CH2Li

NO-C50-NCH3Li

NO-C50-NHLi

Fig. 4: the UV-Visible absorption spectra of pristine C₅₀ fullerene and sandwiched form of it

As it is evident in Fig.4, the UV-Visible absorption spectrum is highly affected by the presence of the donor and acceptor groups. It clearly seen that the C₅₀ has two adjacent absorption bands in about 436 nm and two other adjacent bands in 548 nm. However, presence of donor and acceptor groups considerably enhances the optical properties of it and the number of absorption bands in visible region is noticeably increased. In the all cases, a considerable absorption band was created in higher than the 800 nm, which is located in near IR region. The more considerable results was obtained when the -NCH₃Li group as electron donating group in company with the electron acceptor groups are attached to the C₅₀. In the cases of BH₂-C₅₀-NCH₃Li and NO-C₅₀-NCH₃Li the absorption bands are exist in 1382 and 1373 nm which have notable intensity.

In continue, to explore the influence of the donor and acceptor groups on C₅₀ optical properties, the wavelengths and corresponding oscillator strength for absorption lines of pristine C₅₀ fullerene and all donor-acceptor sandwiched forms of it was recorded. In Tables 3 the wavelengths and corresponding oscillator strengths of UV-Visible absorption for C₅₀ were reported. The wavelengths and corresponding oscillator strengths of UV-Visible absorption for the -BH₂ group as electron acceptor and other electron donor group is reported in Table 4. Similarly the results of wavelengths and corresponding oscillator strengths of UV-Visible absorption for the -NO group as electron acceptor and other electron donor groups is reported in Table 5.

Table3: the wavelengths and corresponding oscillator strength of absorption lines of
pristine fullerene

C50	
λ	f

1	548.49	0.0682
2	548.48	0.0689
3	436.88	0.0799
4	436.88	0.0800

Similar to Fig 4, the data of Table 3, show that the C₅₀ fullerenes have 4 absorption lines in visible region. The λ_{max} for them are about 548 and 436 nm. The wavelengths and corresponding oscillator strength for absorption lines of C₅₀ fullerene, which was sandwiched between the BH2 as electron acceptor and other electron donor groups, is reported.

Table 4: the wavelengths and corresponding oscillator strength for absorption lines of C₅₀ sandwiched between the BH₂ electron acceptor and other electron donor groups

	BH ₂ -C50-CH ₂ Li		BH ₂ -C50-NCH ₃ Li		BH ₂ -C50-NHLi	
	λ	F	λ	F	λ	f
1	857.25	0.009	1382.05	0.0219	1319.53	0.0013
2	771.02	0.010	946.14	0.0015	826.56	0.0019
3	732.40	0.0005	822.23	0.0088	819.35	0.0102
4	593.89	0.0001	706.17	0.0005	706.69	0.0003
5	582.93	0.0174	660.92	0.0003	596.76	0.0009
6	571.48	0.0001	616.12	0.0030	591.33	0.0176
7	555.29	0.0160	595.86	0.0007	565.82	0.0013
8	552.11	0.0001	590.98	0.0165	559.65	0.0003
9	548.05	0.0005	566.10	0.0023	558.73	0.0009
10	543.58	0.0110	557.25	0.0014	553.10	0.0002
11	528.26	0.0057	553.55	0.0003	548.21	0.0051
12	483.56	0.0957	545.19	0.0046	539.51	0.0026
13	467.94	0.0005	524.35	0.0085	526.81	0.0088
14	456.35	0.0004	511.16	0.0054	511.33	0.0067
15	447.64	0.0010	499.46	0.0014	481.25	0.0650
16	442.36	0.0001	481.75	0.0663	476.84	0.0082
17	441.79	0.0001	477.07	0.0029	466.04	0.0031
18	441.22	0.0077	465.51	0.0014	464.32	0.0185
19	429.94	0.0054	463.47	0.0351	461.91	0.0139
20	427.72	0.0066	449.49	0.0016	449.77	0.0035
21	418.97	0.0145	444.25	0.0038	445.14	0.0025
22	414.89	0.0194	438.47	0.0010	440.07	0.0001
23	409.11	0.0219	432.14	0.0032	432.99	0.0052
24	400.91	0.0190	430.23	0.0056	428.92	0.0074

25	400.61	0.0032	428.90	0.0097	418.89	0.0029
26			418.99	0.0034	417.22	0.0112
27			415.54	0.0055	413.14	0.0127
28			411.72	0.0122	409.41	0.0186
29			410.66	0.0146	406.78	0.0154
30			405.53	0.0186	400.36	0.0056
31			401.17	0.0028		
32			400.07	0.0051		

As illustrated in Table 4, it was shown that as consequence of presence of $-BH_2$ groups as electron donor group, the optical properties of C_{50} were enhanced. The number of absorption bands for $BH_2-C_{50}-CH_2Li$, $BH_2-C_{50}-NCH_3Li$ and $BH_2-C_{50}-NHLi$ are 23, 32 and 30 respectively.

It seems that the presence of these donor and acceptor groups considerably relaxes the selection rule of electronic transitions. The absorption bands which observed in 1382 and 1319 nm for $BH_2-C_{50}-NCH_3Li$ and $BH_2-C_{50}-NHLi$ is very interesting.

Similar to Table 4, the results of the wavelengths and corresponding oscillator strengths for absorption bands of the C_{50} attached with the $-NO$ and other electron donor groups in wavelengths greater than 400 nm is gathered in Table 5.

Table 5: the wavelengths and corresponding oscillator strength for absorption lines of C_{50} sandwiched between the $-NO$ electron acceptor and other electron donor groups

	NO- C_{50} - CH_2Li		NO- C_{50} - NCH_3Li		NO- C_{50} - $NHLi$	
	λ	f	λ	f	λ	f
1	1378.55	0.0015	1380.51	0.0260	1372.77	0.0010
2	888.59	0.0110	919.6	0.0005	847.44	0.0108
3	783.7	0.0018	846.62	0.0103	801.72	0.0020
4	732.88	0.0081	754.56	0.0007	757.01	0.0007

5	713.87	0.0004	709.89	0.0005	701.35	0.0003
6	608.38	0.0002	694.44	0.0001	634.8	0.0011
7	600.81	0.0002	628.51	0.0009	587.12	0.0060
8	595.41	0.0073	608.87	0.0032	578.47	0.0004
9	589.42	0.0007	588.5	0.0059	575.43	0.0048
10	580.47	0.0069	579.08	0.0011	571.68	0.0078
11	563.54	0.0235	574.07	0.0117	567.59	0.0010
12	561.37	0.0104	567.3	0.0009	560.74	0.0094
13	555.79	0.0088	566.26	0.0001	552.85	0.0043
14	551.06	0.0014	558.75	0.0096	546.38	0.0051
15	542.17	0.0001	543.93	0.0042	531.2	0.0052
16	512.09	0.0067	529.65	0.0054	522.2	0.0003
17	507.69	0.0001	508.88	0.0012	510.85	0.0010
18	491.24	0.0321	486.57	0.0714	487.68	0.0601
19	487.7	0.0513	479.29	0.0199	480.49	0.0318
20	469.79	0.0007	471.98	0.0077	471.43	0.0080
21	460.36	0.0002	467.1	0.0264	466.17	0.0260
22	455.62	0.0196	462.96	0.0004	460.97	0.0002
23	451.12	0.0059	461.45	0.0014	454.54	0.0048
24	435.56	0.0038	454.16	0.0037	442	0.0104
25	433.37	0.0015	443.15	0.0095	438.77	0.0008
26	431.83	0.0002	439.04	0.0012	435.29	0.0044
27	427.41	0.0069	434.52	0.0038	432.74	0.0045
28	424.69	0.0015	432.28	0.0035	431.73	0.0034
29	420.65	0.0116	426.68	0.0060	427.41	0.0056
30	418.3	0.0054	424.28	0.0026	424.99	0.0031
31	410.75	0.0140	423.21	0.0081	417.34	0.0064
32	407.11	0.0099	417.9	0.0053	415.03	0.0089
33	405.34	0.0133	411.03	0.0135	409.08	0.0148
34	400.96	0.0134	406.98	0.0025	403.65	0.0020
35			402.32	0.0022		

Observing the data represented in Table 5 demonstrates that, similar to $-\text{BH}_2$ group, the optical properties of C_{50} fullerene, was modified in presence of the $-\text{NO}$ group in accompany with other electron donor groups. In this case, the $\text{NO}-\text{C}_{50}-\text{NCH}_3\text{Li}$ molecule has more considerable result which has 35 absorption-lines in visible and near infrared region and has an absorption-line in 1380 nm with notable intensity.

3.4. Nonlinear optical properties

In this section, the values of polarizability (α) and first hyperpolarizability (β_0), which are representative of linear and nonlinear optical properties of nanoclusters, for C_{50} in pristine and substituted forms were computed at CAM-B3LYP/6-311G(d,p) level and presented in Table 6.

Table6. The values of μ , α , and β for C_{50} fullerene and sandwiched forms of it between donor and acceptor groups

Molecule	μ (Deby)	α (a.u)	β (a.u)
C_{50}	0.0004	482	8.0
$BH_2-C_{50}-NHLi$	1.97	471	916
$BH_2-C_{50}-NCH_3Li$	1.74	491	3662
$BH_2-C_{50}-CH_2Li$	1.48	483	1089
$NO-C_{50}-NHLi$	2.93	468	2322
$NO-C_{50}-NCH_3Li$	2.52	489	2734
$NO-C_{50}-CH_2Li$	2.26	479	3066

As represented in Table 6, calculated dipole moment of C_{50} fullerene is very small and equal to 0.0004. On the other hand sandwiching C_{50} between the donor and acceptor groups drastically increases its dipole moments. Between the selected molecules, the $NO-C_{50}-NHLi$ molecule has higher dipole moment. It was observed that almost the same results were obtained for considered molecules. However, the first hyperpolarizability of it is enhanced in presence of donor and acceptor groups. The more improvements in the first hyperpolarizability were obtained in the case of $BH_2-C_{50}-NCH_3Li$ and $NO-C_{50}-NHLi$ molecules.

4. Conclusion

Due to the great importance of fullerenes and their special structure, they have attracted a lot of attention from scientists. One of the common ways to improve the physical and chemical properties of fullerenes is chemical functionalization of them. In present study, the C_{50} fullerene

was used as the source of the π electrons and to enhance its optical properties the electron donor-acceptor groups were used. The results show that the electronic and optical property of C_{50} is considerably enhanced by donor and acceptor group presence. The number of absorption lines in visible region drastically increase and it seems that the selection rule of electronic transition was relaxed. The substituted forms of C_{50} , has numbers of absorption bands in near infrared region, which is very interesting. Most improvement in optical properties was obtained for $BH_2-C_{50}-NCH_3Li$ and $NO-C_{50}-NCH_3Li$ molecules. Finally, the effect of donor and acceptor groups on non-linear optical properties (NLO) was studied and it was shown that the considerable improvement in their NLO properties was seen. Most improvements in NLO response was seen in the $BH_2-C_{50}-NCH_3Li$ and $NO-C_{50}-CH_2Li$ cases.

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AUTHORS DECLARATION

Dear Editor

-Ethical approval

we the undersigned declare that the manuscript entitled **“Improving the electrical and optical properties of C50 fullerene using the Donor-Acceptor groups ”** which sent to your esteemed Journal *“Journal of Molecular Modeling”* is original, has not been published before and is not currently being considered for publication elsewhere.

-Consent to Participate and publish

We would like to draw the attention of the Editor to the following publications of one or more of us that refer to aspects of the manuscript presently being submitted. We wish to confirm that there are no known conflicts of interest associated with this publication.

-Funding

We would like to confirm that there has been no significant financial support for this work that could have influenced its outcome.

-Authors Contribution

We confirm that the manuscript has been read and approved that there are no other persons who satisfied the criteria for authorship but are not listed.

-Availability of data and materials

We confirm that we have given due consideration to the protection of intellectual property associated with this work and that there are no impediments to publication, including the timing of publication, with respect to intellectual property. In so doing we confirm that we have followed the regulations of my institutions concerning intellectual property. We understand that the Corresponding Author is the sole contact for the Editorial process (including Editorial Manager and direct communications with the office). We confirm that we have provided a current, correct email address which is accessible by the Corresponding Author and which has been configured to accept email from.

-Code availability

All calculations were performed with a legally licensed version of the Gaussian program using facilities at the institute of postgraduate studies, University of Malaya, Kuala Lumpur, Malaysia.

Ali Ayoubikaskooli
Hamid Reza Shamlouei

Abdol Mohammad Ghaedi
Yadollah Saghapour